



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 PM UTC

PDB ID : 7JWJ / pdb_00007jwj
Title : Crystal Structure of B17-C1 TCR-H2Db
Authors : Farenc, C.; Rossjohn, J.; Gras, S.; Szeto, C.
Deposited on : 2020-08-25
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

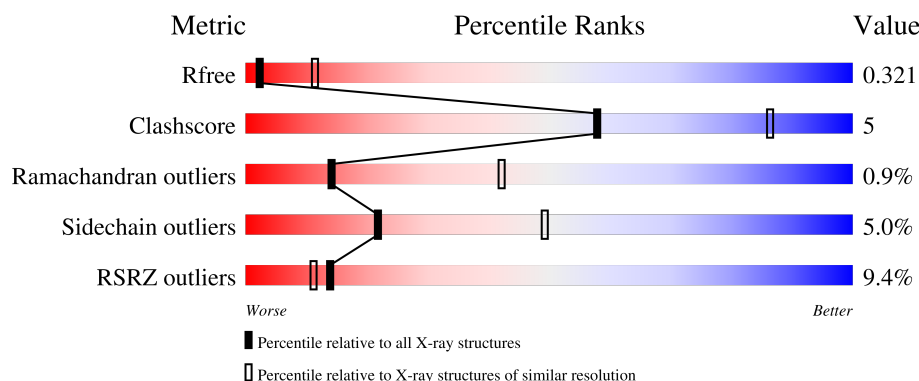
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	11% 65% 9% 27%
2	B	119	6% 62% 18% 18%
3	C	9	11% 89% 11%
4	D	204	9% 80% 15%
5	E	245	4% 85% 12%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6561 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2189	1385	388	407	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	1	0
			810	518	137	148	7			

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			

- Molecule 4 is a protein called B17.C1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	196	Total	C	N	O	S	0	0	0
			1525	942	265	310	8			

- Molecule 5 is a protein called B17.C1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1958	1243	341	365	9			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		

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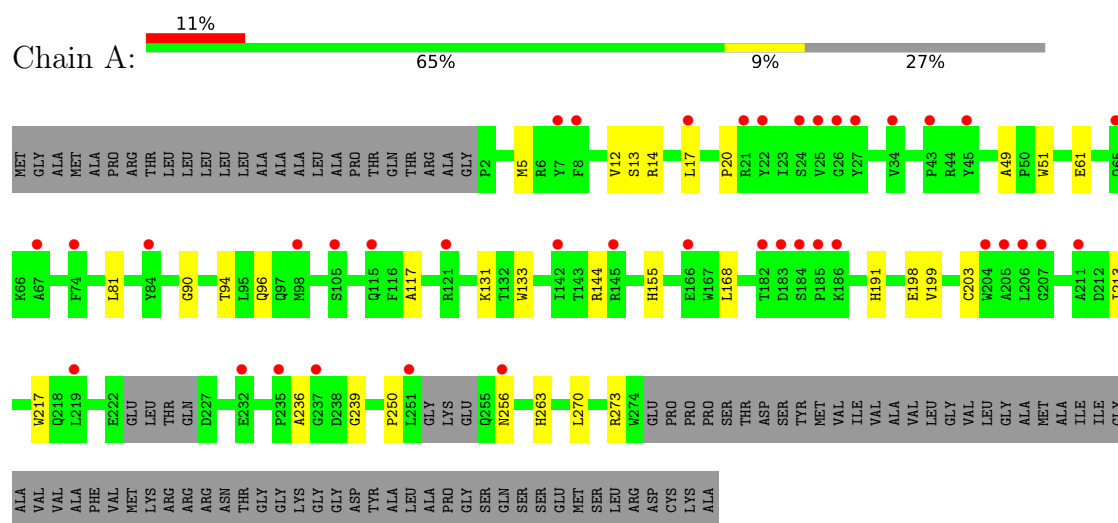
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	E	3	Total 3	O 3	0	0

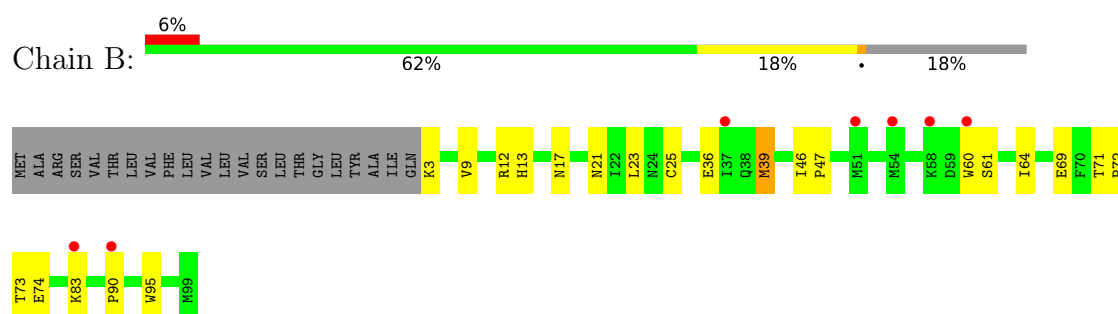
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

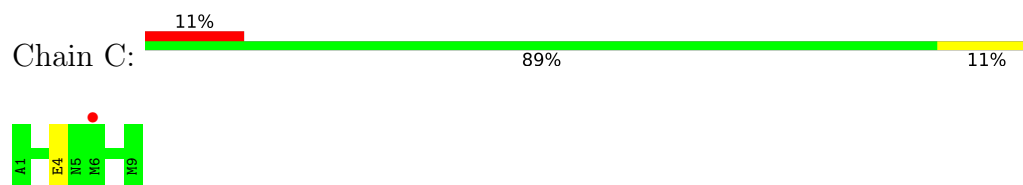
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



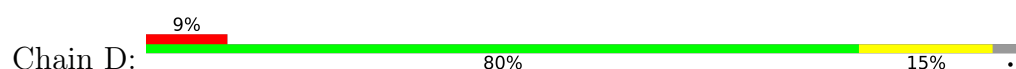
- Molecule 2: Beta-2-microglobulin

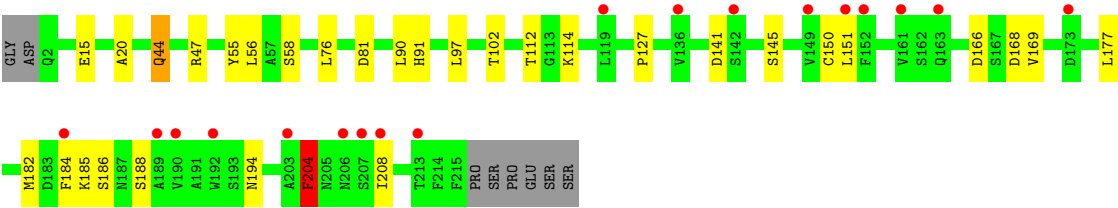


- Molecule 3: Nucleoprotein

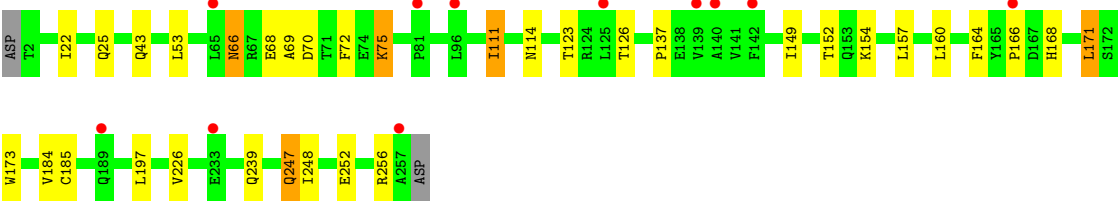
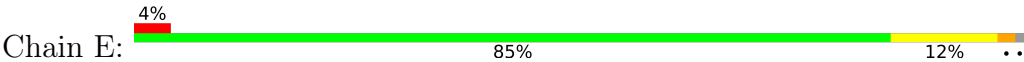


- Molecule 4: B17.C1 TCR alpha chain





● Molecule 5: B17.C1 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.77Å 224.64Å 172.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.25 47.65 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.65-3.25) 99.3 (47.65-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.276 , 0.306 0.290 , 0.321	Depositor DCC
R_{free} test set	952 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	105.5	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6561	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/2253	0.79	0/3057
2	B	0.52	0/836	0.81	0/1132
3	C	0.53	0/68	0.68	0/88
4	D	0.54	0/1552	0.89	1/2098 (0.0%)
5	E	0.52	0/2012	0.81	0/2735
All	All	0.51	0/6721	0.82	1/9110 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	204	PHE	CA-CB-CG	6.08	119.89	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2189	0	2064	17	0
2	B	810	0	787	17	0
3	C	69	0	61	1	0
4	D	1525	0	1454	13	0
5	E	1958	0	1890	15	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
6	E	3	0	0	0	0
All	All	6561	0	6256	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:PHE:HD2	5:E:75:LYS:HZ1	1.16	0.93
2:B:23:LEU:HD11	2:B:95:TRP:CD1	2.05	0.90
2:B:9:VAL:HG12	2:B:95:TRP:HD1	1.38	0.88
4:D:166:ASP:HB3	4:D:169:VAL:HB	1.63	0.81
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.00	0.75
1:A:13:SER:HA	1:A:20:PRO:HB3	1.70	0.74
2:B:23:LEU:HD11	2:B:95:TRP:NE1	2.08	0.68
2:B:83[B]:LYS:HG2	2:B:90:PRO:HB3	1.77	0.66
2:B:9:VAL:HG12	2:B:95:TRP:CD1	2.27	0.64
2:B:17:ASN:HA	2:B:72:PRO:HB2	1.79	0.64
4:D:20:ALA:HB2	4:D:91:HIS:CD2	2.34	0.62
2:B:39:MET:HB3	2:B:46:ILE:HD12	1.81	0.62
1:A:198:GLU:HB2	1:A:250:PRO:HA	1.82	0.60
4:D:141:ASP:HB3	4:D:145:SER:HA	1.83	0.60
5:E:137:PRO:HB3	5:E:164:PHE:HB3	1.84	0.59
1:A:133:TRP:HB2	1:A:144:ARG:HG3	1.83	0.59
5:E:126:THR:HG23	5:E:168:HIS:NE2	2.17	0.59
5:E:173:TRP:CD1	5:E:184:VAL:HG13	2.38	0.58
1:A:14:ARG:HB3	1:A:17:LEU:HB2	1.85	0.57
2:B:36:GLU:HB2	2:B:83[A]:LYS:HB3	1.90	0.54
5:E:43:GLN:HB2	5:E:53:LEU:HD11	1.88	0.54
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.88	0.54
2:B:36:GLU:HB2	2:B:83[B]:LYS:HB2	1.89	0.53
1:A:198:GLU:CB	1:A:250:PRO:HA	2.40	0.51
1:A:13:SER:HA	1:A:20:PRO:CB	2.39	0.51
2:B:13:HIS:ND1	2:B:21:ASN:HA	2.26	0.49
4:D:55:TYR:OH	5:E:114:ASN:O	2.26	0.49
5:E:173:TRP:HD1	5:E:184:VAL:CG1	2.26	0.49
4:D:168:ASP:HB3	4:D:194:ASN:HB3	1.94	0.48
5:E:69:ALA:O	5:E:70:ASP:HB3	2.13	0.48
4:D:177:LEU:HB2	4:D:186:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:LEU:HD23	4:D:90:LEU:HD11	1.95	0.48
1:A:203:CYS:SG	1:A:217:TRP:CZ2	3.08	0.47
4:D:204:PHE:H	4:D:204:PHE:HD1	1.63	0.47
2:B:25:CYS:HB2	2:B:39:MET:HE3	1.97	0.46
4:D:15:GLU:HG3	4:D:127:PRO:HA	1.98	0.46
1:A:191:HIS:CE1	1:A:199:VAL:CG2	2.99	0.45
5:E:171:LEU:HG	5:E:226:VAL:HG22	1.98	0.45
1:A:213:ILE:HD12	1:A:263:HIS:HD2	1.81	0.45
5:E:149:ILE:O	5:E:152:THR:O	2.33	0.45
4:D:44:GLN:HG2	4:D:102:THR:HB	1.99	0.45
5:E:72:PHE:HB2	5:E:75:LYS:NZ	2.32	0.45
4:D:112:THR:HA	5:E:111:ILE:HD12	1.98	0.45
1:A:236:ALA:HB1	2:B:12:ARG:HG3	1.98	0.45
5:E:66:ASN:ND2	5:E:68:GLU:HB2	2.32	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:A:155:HIS:HE1	3:C:4:GLU:O	2.01	0.44
2:B:23:LEU:CD1	2:B:95:TRP:NE1	2.79	0.44
2:B:3:LYS:NZ	2:B:61:SER:HB3	2.32	0.44
5:E:173:TRP:CD1	5:E:184:VAL:CG1	2.99	0.44
1:A:49:ALA:HB1	1:A:51:TRP:CD1	2.54	0.42
1:A:256:ASN:HB3	1:A:273:ARG:HD2	2.01	0.42
1:A:12:VAL:HG22	1:A:94:THR:HG23	2.01	0.42
2:B:71:THR:HA	2:B:72:PRO:HD3	1.95	0.42
2:B:46:ILE:HA	2:B:47:PRO:HD3	1.96	0.41
4:D:151:LEU:HD11	4:D:188:SER:HB2	2.03	0.41
4:D:20:ALA:CB	4:D:91:HIS:CD2	3.03	0.40
5:E:247:GLN:HE21	5:E:247:GLN:HB2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/362 (72%)	248 (95%)	10 (4%)	2 (1%)	16	44
2	B	96/119 (81%)	92 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	194/204 (95%)	175 (90%)	15 (8%)	4 (2%)	5	25
5	E	241/245 (98%)	229 (95%)	11 (5%)	1 (0%)	30	59
All	All	798/939 (85%)	750 (94%)	41 (5%)	7 (1%)	14	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	182	MET
4	D	185	LYS
4	D	114	LYS
4	D	58	SER
5	E	166	PRO
1	A	239	GLY
1	A	90	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/296 (76%)	221 (98%)	5 (2%)	45	65
2	B	92/110 (84%)	87 (95%)	5 (5%)	20	47
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	173/181 (96%)	164 (95%)	9 (5%)	21	48
5	E	215/217 (99%)	198 (92%)	17 (8%)	11	35
All	All	714/812 (88%)	678 (95%)	36 (5%)	22	49

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLU

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Mol	Chain	Res	Type
1	A	81	LEU
1	A	96	GLN
1	A	131	LYS
1	A	270	LEU
2	B	39	MET
2	B	64	ILE
2	B	69	GLU
2	B	73	THR
2	B	74	GLU
4	D	44	GLN
4	D	47	ARG
4	D	56	LEU
4	D	81	ASP
4	D	97	LEU
4	D	150	CYS
4	D	184	PHE
4	D	204	PHE
4	D	208	ILE
5	E	22	ILE
5	E	25	GLN
5	E	66	ASN
5	E	75	LYS
5	E	111	ILE
5	E	123	THR
5	E	154	LYS
5	E	157	LEU
5	E	160	LEU
5	E	171	LEU
5	E	185	CYS
5	E	197	LEU
5	E	239	GLN
5	E	247	GLN
5	E	248	ILE
5	E	252	GLU
5	E	256	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	115	GLN
1	A	155	HIS

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	256	ASN
2	B	67	HIS
4	D	91	HIS
4	D	126	GLN
4	D	187	ASN
4	D	205	ASN
5	E	66	ASN
5	E	84	ASN
5	E	133	ASN
5	E	189	GLN
5	E	198	ASN
5	E	247	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	266/362 (73%)	1.05	39 (14%) 6 5	36, 130, 219, 230	14 (5%)
2	B	97/119 (81%)	0.64	7 (7%) 21 15	69, 158, 170, 174	4 (4%)
3	C	9/9 (100%)	0.77	1 (11%) 10 9	100, 101, 104, 106	0
4	D	196/204 (96%)	0.62	18 (9%) 14 11	75, 101, 145, 150	1 (0%)
5	E	243/245 (99%)	0.34	11 (4%) 38 25	69, 93, 122, 130	1 (0%)
All	All	811/939 (86%)	0.68	76 (9%) 14 11	36, 113, 203, 230	20 (2%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	14.5
1	A	205	ALA	13.7
1	A	185	PRO	11.3
1	A	204	TRP	9.5
1	A	186	LYS	7.0
4	D	161	VAL	6.7
1	A	98	MET	6.4
5	E	257	ALA	4.6
1	A	34	VAL	4.5
1	A	45	TYR	4.4
1	A	24	SER	4.3
4	D	207	SER	4.0
2	B	37	ILE	3.9
4	D	208	ILE	3.9
5	E	166	PRO	3.9
1	A	142	ILE	3.8
1	A	21	ARG	3.8
5	E	142	PHE	3.7
2	B	83[A]	LYS	3.5
5	E	189	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	54	MET	3.5
1	A	7	TYR	3.3
1	A	27	TYR	3.3
4	D	203	ALA	3.2
1	A	219	LEU	3.1
1	A	74	PHE	3.0
1	A	183	ASP	3.0
5	E	233	GLU	3.0
4	D	184	PHE	3.0
1	A	115	GLN	2.9
1	A	237	GLY	2.9
1	A	166	GLU	2.8
1	A	207	GLY	2.8
1	A	22	TYR	2.8
1	A	145	ARG	2.8
1	A	26	GLY	2.8
1	A	84	TYR	2.8
1	A	25	VAL	2.7
2	B	51	MET	2.6
1	A	184	SER	2.6
4	D	206	ASN	2.6
5	E	125	LEU	2.6
4	D	142	SER	2.6
1	A	65	GLN	2.6
4	D	119	LEU	2.6
1	A	105	SER	2.6
4	D	190	VAL	2.5
4	D	152	PHE	2.4
4	D	163	GLN	2.4
2	B	90	PRO	2.4
1	A	67	ALA	2.4
4	D	149	VAL	2.4
5	E	139	VAL	2.4
4	D	151	LEU	2.4
4	D	189	ALA	2.3
3	C	6	MET	2.3
1	A	17	LEU	2.3
1	A	251	LEU	2.3
1	A	235	PRO	2.3
1	A	211	ALA	2.3
2	B	58	LYS	2.3
1	A	232	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	140	ALA	2.2
1	A	43	PRO	2.2
4	D	173	ASP	2.2
1	A	121	ARG	2.2
4	D	213	THR	2.1
5	E	65	LEU	2.1
1	A	256	ASN	2.1
1	A	182	THR	2.1
1	A	8	PHE	2.1
5	E	81	PRO	2.1
2	B	60	TRP	2.1
4	D	136	VAL	2.0
5	E	96	LEU	2.0
4	D	192	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.